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MULTIVARIATE CALIBRATION AND YIELD ESTIMATION

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13. ABSTRACT *(Maximum 200 words)*

Calibration of the linear magnitude-yield relation and estimation of yields from subsequent vector magnitudes is studied from the classical and Bayesian points of view. Calibration regressions are developed using (1) sampled magnitude-yield pairs, (2) sampled pairs and prior information and (3) sampled magnitudes and CORRTEX measurements. Yield estimates and confidence intervals are derived under all three assumptions using the predictive distribution of the observed magnitude. Prior information, such as might be provided by expert panels, is incorporated through distributional assumptions made on the slope-intercept vectors and the yield-adjusted magnitude covariance matrix. A maximum likelihood estimation procedure is derived for the case where CORRTEX yields are available. All methods are illustrated on a population of 16 magnitude pairs (m_b, L_g) and associated announced yields from Semipalatinsk.

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1. Introduction

There are two important problems in monitoring nuclear tests using seismic and other means, *either in a proliferation or treaty monitoring* environment. The first is calibrating an assumed relation between the yield of a nuclear test and a vector of observed magnitudes. For example, we may measure body wave magnitudes, m_b and L_g for a number of nuclear tests and seek to calibrate some function to the observed data which will allow prediction of yield from the magnitude vector. The prediction of yield and its associated uncertainty from observations on a future magnitude vector is the second important problem of interest considered in this report.

To illustrate the nature of the first problem, consider a set of 16 explosions from the Russian site at Semipalatinsk for which yields have been published in Bocharov et al (1989) and Vergino (1989). The data, listed in Table 1 of Section 5, are plotted in Figure 1 where it is fairly clear that a linear model relating both magnitudes to the logarithm of the announced yield would not be unreasonable. The only apparent deviation from linearity is the second event where the m_b value seems out of line. Fitting linear regressions of the two magnitudes on log-yield seems to be a natural way of estimating a calibration relation.

Note that all of these events are from the same region and it is unlikely that monitoring in a proliferation environment could yield such a large calibration set. Furthermore, the slopes and intercepts may vary considerably depending on the location of the event and the location of the network monitoring the event (see Heasler et al, 1990). One would more likely have available a much smaller group of say 5 or 6 vector magnitudes with announced yields as well as some prior information about the nature of the slopes and intercepts. The prior values could based on geologic factors and (or) expert opinion. Given this more limited situation, one could still calculate a classical linear regression of the magnitude vector on yield that would make no use of prior knowledge. One could also ignore the calibration data completely and just use some prior probability distribution for the slope and intercept values based on an uncertainty derived from expert opinion. Alternatively, there is a third Bayesian calibration approach that makes optimal use of both the data and prior information. We will investigate all three approaches in this report.

In the past, there have been close-in hydrodynamic measurements called CORRTEX made on yield; these measurements are generally thought to be more accurate than seismic magnitudes. One can either regard these measurements as highly accurate magnitude surrogates with unit slope and zero intercept or as errors in variables measurements on yield. We discuss a multivariate approach using CORRTEX as an additional measurement

on yield in Section 4.3.

Yield estimation on the basis of the calibration relation derived above is the second important problem we consider in this report. We assume that new yields corresponding to vector magnitudes are fixed and unknown. Then, the predictive distribution (see Atchison and Dunsmore, 1975) of the magnitudes in both the classical and Bayesian frameworks will be functions of the univariate yield. Inverting the predictive magnitude distribution then gives a confidence interval on the unknown future yield. An approach using the classical (non-Bayesian) method of Fieller (1954) in the univariate case was used in Rivers et al (1986) and in Picard and Bryson (1992). The extension of the classical method to the multivariate case is due to Brown (1982). For the Bayesian case, we choose to regard the yields as being fixed and unknown rather than as random with uniform prior distributions as in Brown (1982) and Picard and Bryson (1992). The use of the predictive distribution, without integrating over yields, gives a classical confidence interval rather than the Bayesian interval which would be characterized by the conditional distribution of yield given the magnitude vector in the usual Bayesian approach.

To summarize the approach taken here, we have integrated material from Shumway and Der (1990) and Shumway (1990) with the emphasis changed from monitoring a possible Threshold Test Ban Treaty (TTBT) to monitoring the possible worldwide proliferation of nuclear weapons. A new section is included that covers estimating the yields when CORRTEX measurements are available using maximum likelihood and a Bayesian set of priors for the intercept slope vector. This allows yield estimation using only prior information and no data. To accomplish this, we first introduce the simple linear model relating elements of the magnitude vector to log yield. Included in this specification are the slope and intercept uncertainty, formulated in one case using a bivariate normal prior. and the magnitude uncertainty, formulated using the multivariate inverted Wishart (chi-square) distribution. We then show how the slope and intercept can be calibrated using classical (data only), Bayesian (prior only or prior combined with data) and CORRTEX observations.

A second Bayesian approach is introduced that allows more generality in formulating the prior information on slopes and intercepts but assumes that the covariance matrix is fixed and known. For yield estimation, there is a predictive approach using both the classical and Bayesian assumptions and a Bayesian approach using the empirical Bayes estimators for the slopes and intercepts.

2. Models for Magnitude Data and Prior Information

Figure 1 implies that a linear model relating log-yield to P-wave m_b and L_g magnitudes is reasonable, and evidence from other research (see Ringdal and Marshall, 1989) indicates that other kinds of magnitude measures behave in a similar manner. Then, the linear model relating the vector of p magnitudes from the ith event, $\mathbf{m}_i = (m_{i1}, \ldots, m_{ip})'$, $i = 1 \ldots, N$ to the yields $w_i, i = 1, \ldots, N$ can be written in the form

$$\mathbf{m}_i = \mathbf{a} + \mathbf{b}w_i + \mathbf{e}_i, \tag{2.1}$$

where $\mathbf{a}$ is the px1 vector of unknown intercepts and $\mathbf{b}$ is the px1 vector of slopes. The error vectors $\mathbf{e}_i$ are assumed to be independent zero-mean multivariate normal random variables with common covariance matrix Σ.

It is convenient to collect the sample of observed vector magnitudes in the overall pxN matrix $Y = (\mathbf{m}_1, \ldots, \mathbf{m}_N)$ and to collect the error vectors in a similar matrix, denoted here by $V = (\mathbf{e}_1, \ldots, \mathbf{e}_N)$. Then, defining the matrices

$$X = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ w_1 & w_2 & \cdots & w_N \end{pmatrix} \tag{2.2}$$

and

$$B = (\mathbf{a}, \mathbf{b}) \tag{2.3}$$

leads to writing (2.1) as the overall multivariate linear model

$$Y = BX + V, \tag{2.4}$$

as is given for example, in Anderson (1986, Chapter 8).

If there are a limited number of data points, it may be important to bring in prior information about the intercept and slope components of B and the error covariance matrix Σ . Suppose, for example, that the uncertainty in the covariance matrix Σ can be expressed in terms of the an inverted Wishart distribution (see Anderson, 1984, Section 7.7.1) with parameters m and $\Psi = m\Sigma_0$ where Σ_0 is the prior covariance matrix corresponding to the assumed prior value of Σ and m is the parameter expressing the initial uncertainty. The value of m corresponds roughly to the degrees of freedom or equivalent sample size of the prior information. That is, how large a sample would have been required to produce,for example, the uncertainty of a panel-furnished distribution? The prior distribution of the covariance matrix used is of the form

$$\pi(\Sigma) \propto |\Sigma|^{-\frac{1}{2}(m+p+2)} exp\{-\frac{m}{2} tr\ \Sigma^{-1}\Sigma_0\} \tag{2.5}$$

where $\propto$ denotes ***proportional to*** and tr denotes the trace of a matrix.

In order to illustrate some of the considerations involved in specifying the joint prior distributions described above, consider the case where we record only one magnitude (p=1) and suppose that the distribution of the initial variance is inverted Wishart (chi-square) with m=10 or m=40 and $\sigma_0^2 = .05^2$. Figure 2 shows the probability densities of the standard deviation σ corresponding to the cases m=10 and m=40. It is seen that the choice m=10 corresponds to a wider uncertainty interval (roughly .03 to .12) whereas the choice m=40 narrows the interval (to roughly .04-.07).

One must also specify the uncertainty of the intercept and slope components. The slope and intercept components in $B = (a, b)$ are assumed to be (conditional on Σ) normally distributed. The stacked vector consisting of the rows of B is assumed to be normally distributed with mean components $(\mathbf{a}_0, \mathbf{b}_0)$ and covariance matrix $\Sigma \otimes D_0^{-1}$ where $\otimes$ denotes the Kronecker or direct product. The 2x2 matrix D_0 is chosen to reflect the joint uncertainty structure of $\mathbf{a}$ and $\mathbf{b}$. It corresponds with the joint uncertainty structure of the maximum likelihood estimator, $\hat{B}$, given above in Equation (3.1) for which the comparable stacked vector has covariance matrix $\Sigma \otimes C^{-1}$. For completeness, we give the prior density of the slope-intercept matrix as

$$\pi_1(B|\Sigma) \propto |\Sigma|^{-\frac{1}{2}q} exp\{-\frac{1}{2} tr\ \Sigma^{-1}(B - B_0)D_0(B - B_0)'\} \tag{2.6}$$

In Figure 3, we see the case corresponding to the intercept $\mathbf{a}$ and slope $\mathbf{b}$ having expectations $a_0 = 4.4$ and $b_0 = .9$ and standard deviations .2 and .1. The correlation was taken as -.5 so that the increase in slope must necessarily lead to a decrease in the intercept. In this case, the initial slope uncertainty ranges roughly between .7 and 1.1 with the intercept ranging from 3.9 to 4.9. One would expect that expert input from panels and studies would be used to establish the prior uncertainty regions for $\mathbf{a}, \mathbf{b}$ and Σ. The values chosen here are for illustrative purposes only.

In some cases, it may be useful to consider additional observations or judgements on yield such as would be provided, for example, by CORRTEX monitoring, assumed to be errors-in-variable surrogates for yields through Equation (2.1), i.e.

$$W_i = w_i + \epsilon_i, \tag{2.7}$$

where the errors ϵ_i are assumed independent with differing but known variances σ_i^2. Note that assuming the variances were equal over calibrations would allow estimating them as parameters via maximum likelihood. Consultations with scientific sources indicated that this assumption would not be a reasonable one for measured hydrodynamic yields. It seems natural to model the CORRTEX observation as above but the errors in variable structure introduces a problem in the updating of the slope and intercept matrix. Because of the empirical Bayes nature of the proposed estimators for slope and intercept, there is no term in the equation for their variances that involves the error variance σ_i^2 of the errors in variable measurement (see Shumway, 1991). Therefore, we have taken, as an alternate approach, the point of view that the CORRTEX yield is simply another observation on vector magnitude with mean intercept $a_0 = 0$ and mean slope $b_0 = 1$ with small prior variances. Then, the CORRTEX measurement fits naturally into (2.1) as another component of magnitude.

The incorporation of the CORRTEX yield into the basic model means that we must introduce more flexibility into the priors than is available in those defined in Section 2. For example, the priors there imply that the joint uncertainty in the slope and intercept vector is proportional to the uncertainty in the error in the magnitude observation. It seems desirable to extend the possibilities so that we may have, for example, large uncertainties on the CORRTEX error at the same time we have small uncertainties about the values $a = 0$ and $b = 1$ for CORRTEX. What we give up with this formulation is the ability to be uncertain about the error covariance matrix Σ which can't be easily integrated out. Hence, we will assume that the covariance matrix of each error is known, i.e.

$$cov(\mathbf{e}_i) = \Sigma_i \tag{2.8}$$

In the approach given here, we assume that the intercept and slope vectors $\mathbf{a}$ and $\mathbf{b}$ have a different more general joint normal distribution in that the $2p \times 1$ stacked vector $\beta = (\mathbf{a}', \mathbf{b}')'$ has a normal distribution with mean $\beta_0 = (\mathbf{a}_0', \mathbf{b}_0')'$ and known $2p \times 2p$ covariance matrix

$$\Sigma_\beta = \begin{pmatrix} \Sigma_a & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_b \end{pmatrix}$$

where the covariances of the components $\mathbf{a}$ and $\mathbf{b}$ appear in the $p \times p$ blocks. The form for the prior density function is

$$\pi_2(\beta) \propto exp\{-\frac{1}{2}(\beta - \beta_0)'\Sigma_\beta^{-1}(\beta - \beta_0)\}. \tag{2.9}$$

The problems of interest for the model determined by (2.1) are again calibration and yield estimation. By calibration is meant the estimation of the slope and intercept vectors $\mathbf{b}$ and $\mathbf{a}$ and the covariance matrix Σ in (2.1) from a small data set consisting of paired vector magnitudes and announced yields or yield surrogates. For yield estimation, we seek the best estimator for log yields w for a collection of observed magnitudes. The next section covers calibration.

3. Calibration

In this section, we discuss first in 3.1 the calibration of the regression relation (2.1) using conventional multivariate regression. The classical approach has the advantage that no assumptions are made about $\mathbf{a}$, $\mathbf{b}$ and Σ except that they are fixed and unknown. The disadvantage is that sample sizes are almost always small, leading to considerable uncertainty in the estimated parameter values. In section 3.2 we consider a Bayesian version of regression that allows incorporating prior assumptions about the slope, intercept and yield-adjusted magnitude covariance matrix Σ. If input is allowed as to the probability distributions for the parameters, uncertainties can be tightened up but there is the chance that bad initial assumptions will contaminate results. The possibility of interpreting the yields as errors in variables observations is considered in Section 4.3 under the prior information assumed in the Bayesian approach. In this case, we derive maximum likelihood estimators for the unknown fixed yields in the calibration sample.

3.1 Classical Regression

Under the assumption that the errors in (2.1) are independent zero mean normal variables with $p \times p$ covariance matrix Σ, (see Anderson, 1984) the maximum likelihood estimator for the slope-intercept matrix is

$$\hat{B} = YX'C^{-1} \tag{3.1}$$

where

$$C = XX' \tag{3.2}$$

Noting the partitioned form in (2.2) and (2.3) enables writing (3.1) as

$$\hat{\mathbf{b}} = \frac{\sum_i (w_i - \bar{w})(\mathbf{m}_i - \bar{\mathbf{m}})}{\sum_i (w_i - \bar{w})^2} \tag{3.3}$$

and

$$\hat{\mathbf{a}} = \bar{\mathbf{m}} - \hat{\mathbf{b}}\bar{w} \tag{3.4}$$

where $\bar{w}$ and $\bar{\mathbf{m}}$ are the mean log-yield and magnitudes respectively. In particular, (3.3) and (3.4) show the analogy with the case where $p = 1$. They also emphasize that the results depend on a collection of single log-yield variables, w_i, on the righthand sides. This simplifies the usual multivariate arguments used to invert the predictive distribution for a future unknown yield.

The covariance matrix Σ can be taken as known if sufficient information is available as to the values of the magnitude variances and correlations. One may also compute the maximum likelihood estimator

$$\hat{\Sigma} = (N-2)^{-1}(Y - \hat{B}X)(Y - \hat{B}X)'. \tag{3.5}$$

Note that the above estimators will be well defined only when there are enough observations $N > p + 2$ to make the resulting normal distributions non-singular.

3.2 Bayesian Regression

Now, given that the above prior information can be specified, it is natural that the estimates for the slopes, intercepts and error covariance may change from those specified by the maximum likelihood estimators (3.1) and (3.5) respectively. To handle this, simply take the joint density of Y, B and Σ and derive the joint conditional (on Y) marginal densities of B and Σ. The conditional density of the data Y is the usual likelihood

$$L(Y|B,\Sigma) \propto |\Sigma|^{-\frac{1}{2}N} exp\{-\frac{1}{2} tr\ \Sigma^{-1}(Y - BX)(Y - BX)'\}. \tag{3.6}$$

Taking the posterior means of the density

$$P(B,\Sigma|Y) \propto L(Y|B,\Sigma)\pi(B|\Sigma)\pi(\Sigma)$$

leads to Bayesian estimators proportional to

$$B_N = (\hat{B}C + B_0 D_0)(C + D_0)^{-1} \tag{3.7}$$

where C is defined in (3.2), $B_N = (\mathbf{a}_N, \mathbf{b}_N)$ and

$$\Sigma_N = (m + N + 1 - p)^{-1}\Big(m\Sigma_0 + (N-2)\hat{\Sigma} + (\hat{B} - B_0)(C^{-1} + D_0^{-1})^{-1}(\hat{B} - B_0)'\Big). \tag{3.8}$$

The subscript N differentiates the Bayes estimators from the maximum likelihood estimators $\hat{B}$ and serves as a reminder that the Bayes estimators are based on a sample of size N. These estimators are seen to combine the prior panel information and the data to form a combined estimator for the intercepts, slopes and error covariance matrices.

Using the alternate prior discussed at the end of Section 2 with the prior covariance on the intercept slope vector $\beta = (\mathbf{a}'\mathbf{b}')'$ given as Σ_β, it is convenient to write the model (2.1) in the form

$$\mathbf{m}_i = X_i\beta + \mathbf{e}_i \tag{3.9}$$

where

$$X_i = (I_p, w_i I_p) \tag{3.10}$$

is the $p \times 2p$ partitioned matrix and I_p denotes a $p \times p$ identity matrix. Under the assumptions given above, it is simple to show that for $Y = (\mathbf{m}_1, \ldots, \mathbf{m}_N)$, the Bayesian estimator for the slope and intercept vector, say $\beta_N = E(\beta|Y)$ is

$$\beta_N = \Sigma_N \left(\sum_{i=1}^{N} X_i' \Sigma_i^{-1} \mathbf{m}_i + \Sigma_\beta^{-1} \beta_0 \right), \tag{3.11}$$

where

$$\Sigma_N = \left(\sum_{i=1}^{N} X_i' \Sigma_i^{-1} X_i + \Sigma_\beta^{-1} \right)^{-1} \tag{3.12}$$

is the conditional covariance matrix.

It is clear that there are two routes that one may take towards estimating the slope from an uncalibrated test site. The first is to insist on fully weighting the available observations and use the ordinary multivariate regression estimators given in (3.1) and (3.5) or (3.11) when the covariance matrices of the errors are known. If a reasonable number of calibration events are furnished and if one believes the yields for these events, it is possible that the slope and intercept estimators will be reasonably good; the variances of the estimators can be read from the estimated covariance matrix $\hat{\Sigma} \otimes C^{-1}$. However, there may be compelling reasons for incorporating prior information into the estimation procedure. The first is that there may be considerable geophysical information and expert opinion that can be used to narrow down the possible values for the slope, intercept and error variance. The second reason is that the observed data may have been deliberately modified to contribute to a distorted magnitude-yield picture. The Bayesian solution has the advantage of being able to weight optimally the two components of information contributed by the expert opinion (prior distribution) and the data.

3.3 Empirical Bayes With CORRTEX

We now consider deriving maximum likelihood estimators for the yields $w_1, \ldots, w_N$ under the model given at the ends of section 2 and section 3.3 where the covariance matrix of the errors is assumed known. Consider the joint likelihood of the N magnitudes and hydrodynamic CORRTEX yields, where we assume that the last element of the vector $\mathbf{m}_i$ contains the CORRTEX yield W_i, defined as an observation satisfying (2.7). The likelihood is written as

$$\prod_{i=1}^{N} p(\mathbf{m}_i; w_i) = \prod_{i=1}^{N} \int p(\mathbf{m}_i|\beta, w_i)\pi_2(\beta)\, d\beta \tag{3.13}$$

where $p(\mathbf{m}_i|\beta, w_i)$ denotes the density (conditional on β) of the i^{th} magnitude and $\pi_2(\beta)$ denotes the prior given by (2.9). We assume for convenience that all Σ_i are known. It is clear from (2.9) and (3.9) that $\mathbf{m}_1, \ldots \mathbf{m}_N$ are jointly normal with mean $X_i\beta_0$ and covariance matrix determined by

$$cov(\mathbf{m}_i, \mathbf{m}_j) = \begin{cases} X_i\Sigma_\beta X_i' + \Sigma_i, & \text{if } i = j \\ X_i\Sigma_\beta X_j', & \text{if } i \neq j. \end{cases}$$

The joint likelihood (3.13) is seen from the form of X_i in (3.10) to be a highly nonlinear and intractable function of the unknown log yields $w_1, \ldots, w_N$ and we consider maximizing it by indirect means.

The EM algorithm, see Dempster, Laird and Rubin (1977) offers a considerable simplification to the usual nonlinear optimization approaches. If we were to observe the vector β, the complete-data log-likelihood for this problem would be of the form

$$\begin{aligned} \log L' \propto & -\log|\Sigma_\beta| - \frac{1}{2}(\beta - \beta_0)'\Sigma_\beta^{-1}(\beta - \beta_0) \\ & - \frac{N}{2}\sum_{i=1}^{N} \log|\Sigma_i| - \sum_{i=1}^{N}(\mathbf{m}_i - X_i\beta)'\Sigma_i^{-1}(\mathbf{m}_i - X_i\beta) \end{aligned} \tag{3.14}$$

In order to maximize (3.13), the EM algorithm defines an iterative sequence consisting of maximizing successively $E(\log L'|Y)$. For this to work, we need expressions for $E(\beta|Y)$ and $cov[\beta|Y]$ which are available through Equations (3.11) and (3.12). Then, define $\beta_N = (\mathbf{a}_N', \mathbf{b}_N')'$ and the partitioned conditional covariance matrix

$$\Sigma_{N\beta} = \begin{pmatrix} \Sigma_{Na} & \Sigma_{Nab} \\ \Sigma_{Nba} & \Sigma_{Nb} \end{pmatrix}$$

where the covariances of the components $\mathbf{a}_N$ and $\mathbf{b}_N$, derived from (3.12), appear in the $p \times p$ blocks. To obtain the terms in the expanded form of $E(\log L'|Y)$, write

$$\begin{aligned} E(\mathbf{b}'\Sigma_i^{-1}\mathbf{b}|Y) &= tr\{\Sigma_i^{-1}E(\mathbf{b}\mathbf{b}'|Y)\} \\ &= tr\{\Sigma_i^{-1}(\mathbf{b}_N\mathbf{b}_N' + \Sigma_{Nb})\} \\ &= \mathbf{b}_N'\Sigma_i^{-1}\mathbf{b}_N + tr\{\Sigma_i^{-1}\Sigma_{Nb}\} \end{aligned}$$

and

$$E[\mathbf{b}'\Sigma_i^{-1}(\mathbf{m}_i - \mathbf{a})|Y] = \mathbf{b}_N'\Sigma_i^{-1}\mathbf{m}_i - tr\{\Sigma_i^{-1}\Sigma_{Nab}\}$$

Substituting the above into the complete-data log likelihood yields the estimator

$$w_{i*} = \frac{\mathbf{b}_N'\Sigma_i^{-1}(\mathbf{m}_i - \mathbf{a}_N) - tr\{\Sigma_i^{-1}\Sigma_{Nab}\}}{\delta_{Ni}^2 + tr\{\Sigma_i^{-1}\Sigma_{Nb}\}} \tag{3.15}$$

where

$$\delta_{Ni}^2 = \mathbf{b}_N'\Sigma_i^{-1}\mathbf{b}_N. \tag{3.16}$$

The above equations suggest the following iterative procedure for computing the maximum likelihood estimators.

1. Set the initial yield estimates at the CORRTEX estimates $W_i, i = 1, \ldots, N$
2. Evaluate β_N and Σ_N using Equations (3.11), (3.12) and the current estimated log-yields.
3. Adjust the log-yields using Equations (3.15)-(3.16).
3. Return to Step 2. until convergence.

It is clear that the approach of this section generates *empirical Bayes* estimators for the slope-intercept vector β since the conditional expectations are evaluated at *estimated yields*. These empirical Bayes estimators are functions of the maximum likelihood yield estimators and will have variances that increase as the variances of the maximum likelihood estimators. The problem with the maximum likelihood estimators is that there are as many

unknown yields as there are vector observations so that an asymptotic result will not be available.

This completes the specification of the method for estimating the slope and intercept vectors along with the error covariance matrix using classical and Bayes regression procedures. In the next section, we consider the problems involved in estimating a future unknown yield using the new magnitude vector and the calibrated regressions derived here.

4. Yield Estimation and Uncertainties

We concentrate now on the problem of inferring the yield when the new magnitude vector $\mathbf{m}$ is given as

$$\mathbf{m} = \mathbf{a} + \mathbf{b}w + \mathbf{e}$$

That is, we are interested in solving the above for the yield 10^w given an observation on a new magnitude. Of course, it is quite obvious that given a fixed known $\mathbf{a}$ and $\mathbf{b}$ and the covariance matrix Σ, the maximum likelihood estimator for the log-yield

$$\hat{w} = \frac{\mathbf{b}'\Sigma^{-1}(\mathbf{m} - \mathbf{a})}{\mathbf{b}'\Sigma^{-1}\mathbf{b}} \tag{4.1}$$

is called for because it is unbiased and has variance

$$\sigma_{\hat{w}}^2 = \frac{1}{\mathbf{b}'\Sigma^{-1}\mathbf{b}}. \tag{4.2}$$

For example, in the most trivial case, with independent magnitudes, one obtains the weighted estimator

$$\hat{w} = c_1(m_1 - a_1) + c_2(m_2 - a_2)$$

where

$$c_i = \frac{\frac{b_i^2}{\sigma_i^2}}{\frac{b_1^2}{\sigma_1^2} + \frac{b_2^2}{\sigma_2^2}},$$

often referred to as the *unified yield estimator*.

Furthermore, in the general case given above, there is a 95% confidence interval of the form $\hat{w} \pm 1.96\sigma_{\hat{w}}$. Since w denotes log-yield, say $\log y$, the limits expressed in terms of yield y are (U^{-1}, U) where

$$U = 10^{1.96\sigma_{\hat{w}}} \tag{4.3}$$

is the so-called *uncertainty factor*. It is convenient because the lower and upper limits for yield are obtained by dividing or multiplying the estimated yield by the uncertainty factor.

The difficulties associated with using the simple inverted unified estimator above when **a** and **b** are estimated from calibration data have been discussed at length in the statistical literature (for example, see Brown, 1982, Hoadley, 1970, Oman, 1988, Picard and Bryson, 1989) and we will only say that even under joint normality of $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$, the problem is intractable for the direct estimator given in (4.1). An approach that focuses on the use of the predictive distribution of **m** to derive confidence intervals in the classical case and prediction intervals in the Bayesian case has been given by Brown (1982). We use Brown's method when a calibration set is available and no prior information can be assumed for the slope-intercept and covariance parameters. This corresponds to the calibration information available from the regression approach described in Section 3.1. This method, which is essentially a generalization of that given by Fieller (1954) is reviewed in Section 4.1.

Prior information from expert panels or other sources can be used to incorporate distributional assumptions about the uncertainty of the slope-intercept matrix B and the covariance matrix Σ as in Section 3.2. Brown (1982) describes a fully Bayesian approach that sets a prior distribution on the log-yield w as well and then computes probability intervals from the posterior distribution of w. For example, Picard and Bryson (1992) follow this approach with a uniform distribution assumed a-priori for log-yield. The posterior distribution of log-yield must then be computed by numerical integration methods. An alternate approach, that retains the Bayesian flavor, is to retain the assumption that yields are fixed unknown constants and to carry through the process of inverting the predictive distribution of magnitude as in the classical Fieller methodology. The intervals obtained then have the same interpretation as do the classical ones. This approach, which is essentially new, is given in Section 4.2.

Finally, in the approach incorporating CORRTEX measurements given in Section 3.3, we obtain maximum likelihood estimators for the slope-intercept matrix B which can be used as inputs to estimate yield using a modified version of Equation (4.1). We discuss this approach in Section 4.3.

4.1 Classical Prediction Intervals

We develop a classical interval for a new observation by noting that under the assumptions of Section 3.1, with $\mathbf{m}$ a new magnitude vector and the new unknown yield w, the distribution of the residual

$$\mathbf{m} - \hat{\mathbf{a}} - \hat{\mathbf{b}}w$$

is multivariate normal with mean $\mathbf{0}$ and covariance matrix $(1 + q(w))\Sigma$ where

$$q(w) = (c^{11} + 2c^{12}w + c^{22}w^2) \tag{4.4}$$

with c^{ij} denoting the ij^{th} element of C^{-1}. It is also the case that the residual is independent of $(N-2)\hat{\Sigma}$, which has the Wishart distribution with N-2 degrees of freedom. Then, the quadratic form in the residuals with the inverse of the covariance matrix $(1 + q(w))\hat{\Sigma}$ in the middle has Hotellings T^2 distribution as in Anderson (1984, p. 163) or Brown (1982). Hence, the resulting inequality

$$\frac{(\mathbf{m} - \hat{\mathbf{a}} - \hat{\mathbf{b}}w)'\hat{\Sigma}^{-1}(\mathbf{m} - \hat{\mathbf{a}} - \hat{b}w)}{(1 + q(w))} \leq K_{p,N}(\alpha) \tag{4.5}$$

involving the quadratic form in the residuals can be inverted to obtain a $100(1-\alpha)\%$ confidence interval. The constant is

$$K_{p,N}(\alpha) = \frac{p(N-2)}{(N-p-1)} F_{p,N-p-1}(\alpha), \tag{4.6}$$

with $F_{p,N-p-1}(\alpha)$ denoting the $(1-\alpha)$ critical point on the F distribution with p numerator and N-p-1 denominator degrees of freedom. We obtain the $(1-\alpha)$ level confidence interval as

$$\frac{d}{c} \pm L \tag{4.7}$$

where

$$L = \frac{\sqrt{d^2 - ce}}{c} \tag{4.8}$$

defines the upper and lower limit with

$$c = \hat{\mathbf{b}}'\hat{\Sigma}^{-1}\hat{\mathbf{b}} - c^{22}K_{p,N}(\alpha), \tag{4.9}$$

$$c = \hat{\mathbf{b}}'\hat{\Sigma}^{-1}\hat{\mathbf{b}} - c^{22}K_{p,N}(\alpha), \tag{4.9}$$

$$d = \hat{\mathbf{b}}'\hat{\Sigma}^{-1}(\mathbf{m} - \hat{\mathbf{a}}) + c^{12}K_{p,N}(\alpha) \tag{4.10}$$

and

$$\epsilon = (\mathbf{m} - \hat{\mathbf{a}})'\hat{\Sigma}^{-1}(\mathbf{m} - \hat{\mathbf{a}}) - (1 + c^{11})K_{p,N}(\alpha) \tag{4.11}$$

The confidence intervals, derived by Brown (1982), are the exact analogues of the univariate intervals first given by Fieller (1954). As in the univariate case, the intervals may be open, but this only occurs when the slope vectors are not significantly different from zero at level α. Oman (1988) has proposed an alternative procedure based on geometric arguments when there is a strong chance that the intervals above might be degenerate.

It should be noted that the interval in (4.7) is for log-yield; the interval on yield would be obtained by inverting the limits given by (4.7). By analogy with (4.3), we define the uncertainty number

$$F = 10^{L}. \tag{4.12}$$

Strictly speaking, this requires using d/c as the estimator for log-yield but we will customarily use the slight modification of this implied by Equation (4.1) which does not depend on the α level chosen for the confidence.

4.2 Predictive Bayes Methods

We may also look at deriving posterior predictive intervals under the assumption that only prior information is available in the form of the joint normal inverted Wishart priors on B and Σ in Section 2. Now, denoting the prior inverted Wishart distribution on Σ as $\pi(\Sigma)$ and the conditional density of the intercept and slope matrix B by $\pi(B|\Sigma)$ as before, we may write the posterior predictive density of $\mathbf{m}$ as

$$P(\mathbf{m}) = \int p(\mathbf{m}|B,\Sigma)\pi_1(B|\Sigma)\pi(\Sigma)\, dB\, d\Sigma \tag{4.13}$$

where we integrate first over B and then over Σ. The result leads to a multivariate t distribution for $\mathbf{m}$ (see, for example, Anderson, 1984, p. 283). This implies that the quadratic form in the multivariate t density (involving the residuals $(\mathbf{m} - \mathbf{a}_0 - \mathbf{b}_0 w)$ and the inverse of a particular covariance matrix) has the F distribution. The resulting interval is exactly in the form of (4.8) with

$$c = \mathbf{b}_0'\Sigma_1^{-1}\mathbf{b}_0 - d_0^{22}K_{p,m}(\alpha), \tag{4.14}$$

$$d = \mathbf{b}_0'\Sigma_1^{-1}(\mathbf{m} - \mathbf{a}_0) + d_0^{12}K_{p,m}(\alpha) \tag{4.15}$$

and

$$e = (\mathbf{m} - \mathbf{a}_0)'\Sigma_1^{-1}(\mathbf{m} - \mathbf{a}_0) - (1 + d_0^{11})K_{p,m}(\alpha), \tag{4.16}$$

where d_0^{ij} is the ijth element of D_0^{-1},

$$\Sigma_1 = \frac{m\Sigma_0}{(m-p+1)} \tag{4.17}$$

and

$$K_{p,m}(\alpha) = pF_{p,m-p+1}(\alpha) \tag{4.18}$$

The uncertainty number is computed as before using (4.12) with the modified definitions of the constants c, d and e.

Finally, we look at the case where both data and prior information are available. This means that we introduce the joint likelihood of the calibration data Y in the equation for the posterior predictive density. This leads to

$$P(\mathbf{m}|Y) = \int p(\mathbf{m}|B,\Sigma)L(Y|B,\Sigma)\pi_1(B|\Sigma)\pi(\Sigma)\;dB\;d\Sigma \tag{4.19}$$

where $L(Y|B,\Sigma)$ denotes the likelihood as the usual conditional density of the data given the parameters. Performing the above integration leads to the posterior t-distribution as before and the interval (4.8) obtains again with the values

$$c = \mathbf{b}_N'\Sigma_N^{-1}\mathbf{b}_N - d_N^{22}K_{p,m,N}(\alpha), \tag{4.20}$$

$$d = \mathbf{b}_N'\Sigma_N^{-1}(\mathbf{m} - \mathbf{a}_N) + d_N^{12}K_{p,m,N}(\alpha) \tag{4.21}$$

and

$$e = (\mathbf{m} - \mathbf{a}_N)'\Sigma_N^{-1}(\mathbf{m} - \mathbf{a}_N) - (1 + d_N^{11})K_{p,m,N}(\alpha). \tag{4.22}$$

where $B_N = (\mathbf{a}_N, \mathbf{b}_N)$ so that $\mathbf{a}_N$ and $\mathbf{b}_N$ can be picked out of the Bayesian regression matrix computed in Equation (3.9) in Section 3.2 and Σ_N is defined in (3.10). In these expressions d_N^{ij} denotes the ij^{th} element of D_N^{-1} where

$$D_N = C + D_0 \tag{4.23}$$

and the constant is

$$K_{p,m,N}(\alpha) = pF_{p,m+N+1-p}(\alpha). \tag{4.24}$$

4.3 Predictive Yield Estimation With CORRTEX

In Section 3.3, we derived maximum likelihood estimators for the yields in a calibration sample using CORRTEX yields as the last magnitude observation. This gave empirical Bayes estimators for the slope-intercept vector β_N and its covariance matrix Σ_N as in Equations (3.11) and (3.12) where we evaluate those equations at the estimated log-yields in the calibration sample. Suppose we denote these empirical Bayes estimators by $\hat{\beta}_N$ and $\hat{\Sigma}_N$ respectively. We want to be able to develop an estimator of a single new yield, given an observation vector of magnitudes and a CORRTEX yield of the form

$$\mathbf{m} = \mathbf{a} + \mathbf{b}w + \mathbf{e} \tag{4.25}$$

where $\mathbf{e}$ is assumed to have covariance matrix Σ that is known.

The posterior predictive distribution under the current model that uses the prior density $\pi_2(\beta)$ is difficult to invert in order to derive a confidence interval for the yield measurement as was done in Section 4.2 under the prior density $\pi_1(B|\Sigma)$. However, it would be natural to use an estimator like (4.1) in this case and we consider using (4.1) evaluated at the Bayes estimators $\mathbf{a}_N, \mathbf{b}_N$, leading to

$$\hat{w} = \frac{\mathbf{b}_N'\Sigma^{-1}(\mathbf{m} - \mathbf{a}_N)}{\mathbf{b}_N'\Sigma^{-1}\mathbf{b}_N} \tag{4.26}$$

We can show that, conditional on the calibration data Y, $E(\hat{w}|Y) = w$ and that

$$E[(\hat{w} - w)^2|Y] = \frac{q(w)}{\delta_N^4},$$

where

$$\delta_N^2 = \mathbf{b}_N'\Sigma^{-1}\mathbf{b}_N \tag{4.27}$$

and $q(w)$ is a quadratic form in w. The posterior distribution is normal and we can solve the quadratic equation

$$\frac{(\hat{w} - w)^2\delta_N^2}{q(w)} \leq z_{\frac{\alpha}{2}}^2$$

for w, where $z_{\frac{\alpha}{2}}$ denotes the upper $100(1 - \frac{\alpha}{2})$ percentile on the standard normal distribution. We will use $\alpha = .025$ in agreement with the standard used in previous yield calculations.

The above algebra leads to a posterior confidence interval of the form (4.7) where

$$c = 1 - K_\alpha^2 \mathbf{b}_N' \Sigma^{-1} \Sigma_{Nb} \Sigma^{-1} \mathbf{b}_N \tag{4.28}$$

$$d = \hat{w} - K_\alpha^2 \mathbf{b}_N' \Sigma^{-1} \Sigma_{Nab} \Sigma^{-1} \mathbf{b}_N, \tag{4.29}$$

and

$$e = \hat{w}^2 - K_\alpha^2 (\delta_n^2 + \mathbf{b}_N' \Sigma^{-1} \Sigma_{Na} \Sigma^{-1} \mathbf{b}_N), \tag{4.30}$$

with

$$K_\alpha = \frac{z_{\frac{\alpha}{2}}}{\delta_N^2} \tag{4.31}$$

The uncertainty factors are computed as before, using Equation (4.12).

The practical application of this approach would use an initial set of CORRTEX yields to derive yield estimators using the maximum likelihood procedure of Section 3.3. This also yields the empirical Bayes estimators $\hat{\mathbf{a}}_N$ and $\hat{\mathbf{b}}_N$ for the intercept and slope vectors along with the estimated covariance matrix $\hat{\Sigma}_N$. Then, new yields can be estimated using Equation (4.26) with only seismic values or with combined new seismic and CORRTEX measurements. If only seismic values are available, simply use the submatrices and subvectors without the CORRTEX parts for the estimation procedure.

5. Calibration and Estimation: An Example

In order to give a simple example illustrating the computations involved in the various techniques developed here, we consider a set of 16 Semipalatinsk events for which yields were published in Bocharov et al (1989) and Vergino (1989). For this set of 16 events, we obtained the network averaged body wave magnitudes m_b, corrected for receiver terms as well as the near-source focusing and defocusing effects from Jih and Shumway (1991). The second component that may be useful is root mean squared error computed from L_g magnitudes at a network of Soviet stations at regional distances (1000-4000 km) as given by Israelsson (1991). The 16 events, along with dates are shown in Table 1 below.

Table 1: Magnitudes and Announced Yields From 16 Explosions

Event No.	Date	m_b	L_g	Announced Yield
1	03/20/66	5.853	6.048	100
2	05/07/66	4.456	4.889	4
3	09/29/68	5.641	5.801	60
4	07/23/69	5.186	5.427	16
5	11/30/69	5.945	6.024	125
6	12/28/69	5.660	5.707	46
7	04/25/71	5.826	5.946	90
8	06/06/71	5.319	5.369	16
9	10/09/71	5.136	5.192	12
10	10/21/71	5.341	5.479	23
11	02/10/72	5.289	5.369	16
12	03/28/72	4.984	4.982	6
13	08/16/72	4.921	4.948	8
14	09/02/72	4.602	4.659	2
15	11/02/72	6.160	6.158	165
16	12/06/72	5.983	6.111	140

The magnitudes are plotted against the log-yields, w in Figure 1 and we note the excellent agreement with the linear model (2.1). The exception is the m_b value for the second event which seems low compared to the L_g and the other points. The sample computations here will assume that the magnitude vector and yield values are available for the first six events (above the line in the table) and these six events form the calibration

set. The symbols for the six events are shaded in Figure 1 and we see that they cover a reasonable range of yields.

We assume also that prior information in the form of expert opinion puts the intercepts of the two lines at 4.4 and the slopes at .9. The uncertainties are defined as in Section 2 by assigning standard deviations of .2 to the intercept vectors, .1 to the slope vectors and a correlation of $-.5$ between the intercept and slope. We always assume that the m_b and L_g yield adjusted magnitudes have standard deviations .05 and .03 respectively with correlation .3. This matrix becomes Σ_0 in the Bayesian approach defined by the first set of priors given in (2.5) and (2.6). In this formulation, the announced yields play the part of the known w_i needed for the approach leading to (3.7) and (3.8). Figure 1 shows the regression line at the expected values and it is clear that it lies above the line that might be implied by the data. Inferring yields from this line will lead to severe underestimates. Figure 2 shows the uncertainty region for the intercept and slope;the intercept is between 3.9 and 4.9 approximately 95% of the time with the comparable assumptions on slope involving the interval .65 to 1.15. The assumed correlation (slope increases as the intercept gets smaller) of -.5 restricts this variation somewhat.

In the case where we wish to incorporate CORRTEX values, it seems reasonable to regard the observation on CORRTEX yield as another element in the magnitude vector with $a_0 = 0$ and $b_0 = 1$. Then, the prior distribution given by (2.9) has three components and we may assigned the prior standard deviations of intercept and slope for the CORRTEX magnitude to be a small number (.03 in the present example) with no correlation between the intercept and slope. The matrix Σ_β in (2.9) is a 6×6 matrix.

Table 2 below shows the estimated intercepts and slopes for various methods. The first two lines are the result of simple multivariate regressions not involving the use of prior information. This is the methodology of Section 3.1 and we see that the calibration regression on the first six events differs somewhat from the regression on all 16 events. In particular, the low m_b value pulls the intercept down to 3.92 and increases the slope to .98. The regression on the full set of 16 events gives a more representative line. This shows how far wrong one can go when there is a presumed outlier and we depend on the small calibration sample.

Table 2: Estimated Slopes and Intercepts for Semipalatinsk

	Intercepts		Slopes	
	M_b	L_g	M_b	L_g
Data (16 events)	4.22	4.34	.83	.83
Data (6 events)	3.92	4.45	.98	.77
Bayes Prior	4.40	4.40	.90	.90
Bayes-Data (6 events)	3.97	4.43	.96	.78
Bayes-CORRTEX (6 events)	3.97	4.45	.96	.78

The pure Bayes approach calibrates with the assumed prior distribution and these prior assumptions are reproduced in row 3 of Table 2. Combining the prior assumptions with the first 6 calibration events again pulls the m_b intercept down and the slope up but the L_g slope and intercept are quite close to what obtains for the entire 16 points. All three methods give nearly the same answer when applied to the calibration set.

For the CORRTEX based estimator, we use the empirical Bayes estimators from Equation (3.11), with yields evaluated by the maximum likelihood procedure of Section 3.3. The uncertainties are evaluated using Equation (3.12) and lead to the estimated standard deviations $.06, .04, .009, .04, .02, .009$ for $(a_1, a_2, a_3, b_1, b_2, b_3)$ with correlations $-.95$ between a_1, b_1 and a_2, b_2 and $.27$ between a_1, a_2 and between b_1, b_2. The pairs a_1, b_2 and a_2, b_1 were negatively correlated $(-.26)$ and all other posterior correlations were zero.

The result of applying the methodology of Section 3 to get yield estimators for Events 7-16 are shown in Table 3. One can compare the estimated yields with the announced yields to estimate how well each method works. The data-driven estimator is discussed in Section 4.1. The estimator is (4.1) evaluated at $\hat{\mathbf{a}}, \hat{\mathbf{b}}$ and the endpoints of the confidence interval determine the uncertainty number using (4.8)-(4.12). The pure Bayes estimator involves only prior information and the interval defined by (4.14)- (4.18) with the estimator computed by evaluating (4.1) at $\mathbf{a}_0, \mathbf{b}_0$. Combining data and the prior information gives the Bayes-data estimator by evaluating (4.1) at $\mathbf{b}_N, \mathbf{a}_N$ and using the confidence intervals defined in (4.20)-(4.24).

Table 3: Yield Estimation Results for Semipalatinsk
(6 calibration events)

Event	Yield	Data Driven	Pure Bayes	Bayes-Data	CORRTEX
7	90	90*(2.01)	53(2.39)	87(1.61)	86(1.36)
8	16	18(1.85)	12(2.28)	17(1.60)	17(1.30)
9	12	11(1.86)	7(2.28)	10(1.63)	11(1.28)
10	23	23(1.94)	15(2.24)	23(1.59)	23(1.31)
11	16	18(1.89)	12(2.27)	17(1.60)	17(1.30)
12	6	6(1.75)	4(2.33)	6(1.68)	6(1.26)
13	8	5(1.82)	4(2.33)	5(1.69)	6(1.26)
14	2	2(1.73)	1(2.48)	2(1.83)	2(1.22)
15	165	185(2.12)	98(2.56)	170(1.66)	165(1.39)
16	140	145(2.07)	81(2.47)	140(1.65)	135(1.38)

* Uncertainty factors shown in ( )

The results make it clear that the pure Bayes approach goes wrong because of the choice of a slightly erroneous prior; all yields are underestimated although the uncertainty number is large enough to put all of the announced yields in the predicted uncertainty region. The data-driven regression estimator does reasonably well except for overestimating the two highest yields; again the uncertainty intervals include the true values. Both the Bayes-data and CORRTEX methods do quite well. The Bayes-CORRTEX estimator should do well since there is an extra observation in the vector. For the particular example given here, the Bayes-CORRTEX method assigned weighting coefficients .21, .60, .33 to m_b, L_g and the CORRTEX yield respectively.

6. Discussion

There are many plausible approaches to calibration and estimation in the multivariate case. One must not only be prepared to work with calibration data when it is available but must be willing to develop a yield estimator when no calibration data is provided. It is the second of these two situations that may pertain more often in the current testing environment where monitoring worldwide proliferation is of primary interest. In such an environment, the use of prior information provided by expert panels and by seismic studies of different regions of the earth becomes paramount. The emphasis shifts from an approach that is heavily weighted towards calibration from samples, possibly involving CORRTEX yields, to one that is oriented towards formulating more accurate prior distributions. Because of the emphasis up to this point on the monitoring of a threshold test ban treat (TTBT), the research summarized in this report concentrates on the sampled data approach.

However, it should be pointed out that the predictive Bayes method discussed at the beginning of Section 4.2 is an example of an approach that uses only prior information and needs no calibration sample. The specification of the prior information involves expressing the joint uncertainty in the slope-intercept vectors in terms of a multivariate normal distribution. The mean value of this *multivariate normal* $(\mathbf{a}_0, \mathbf{b}_0)$ *contains* the expected slopes and intercepts whereas the uncertainty is specified through a covariance matrix. Geometrically this involves being able to intuitively choose elliptical uncertainty contours of the form given in Figure 3 that express our prior information about the slope and intercept.

The slope-intercept prior is proportional to the yield- adjusted magnitude covariance matrix which may also be subject to some uncertainty. This is expressed through the inverted Wishart distribution with a specified prior covariance matrix given by Σ_0. The marginal distributions behave like inverted chi- squared distributions with the uncertainty specified by the degree of freedom parameter m. Although the densities are restricted in some sense, they tend to emulate what one might regard as reasonable prior specifications for uncertainty about the parameter Σ.

If the above prior densities are not flexible enough, the approach involving the second set of priors given by Equation (2.9) can be applied. This does impose the restriction that we must be willing to fix the yield adjusted magnitude covariance matrix at some known value. This set of priors seems to be the only realistic way that one can incorporate the errors in variable observation on CORRTEX into the magnitude vector. The posterior variances of the slope-intercept vector will be weighted properly by the CORRTEX variance in this particular configuration.

Unfortunately, any Bayes approach involves the risk of using an incorrect prior so that the estimated posterior yield might be quite far off. However the uncertainty factors will increase in proportion to the variance covariance structures of the slope-intercept vectors and the yield-adjusted magnitude vector. Therefore, the overall statements including the uncertainty factor will include the true yield 95% of the time if the uncertainty of the prior intercepts and slopes in assigned in a realistic fashion. This was seen in the example shown in Table 3.

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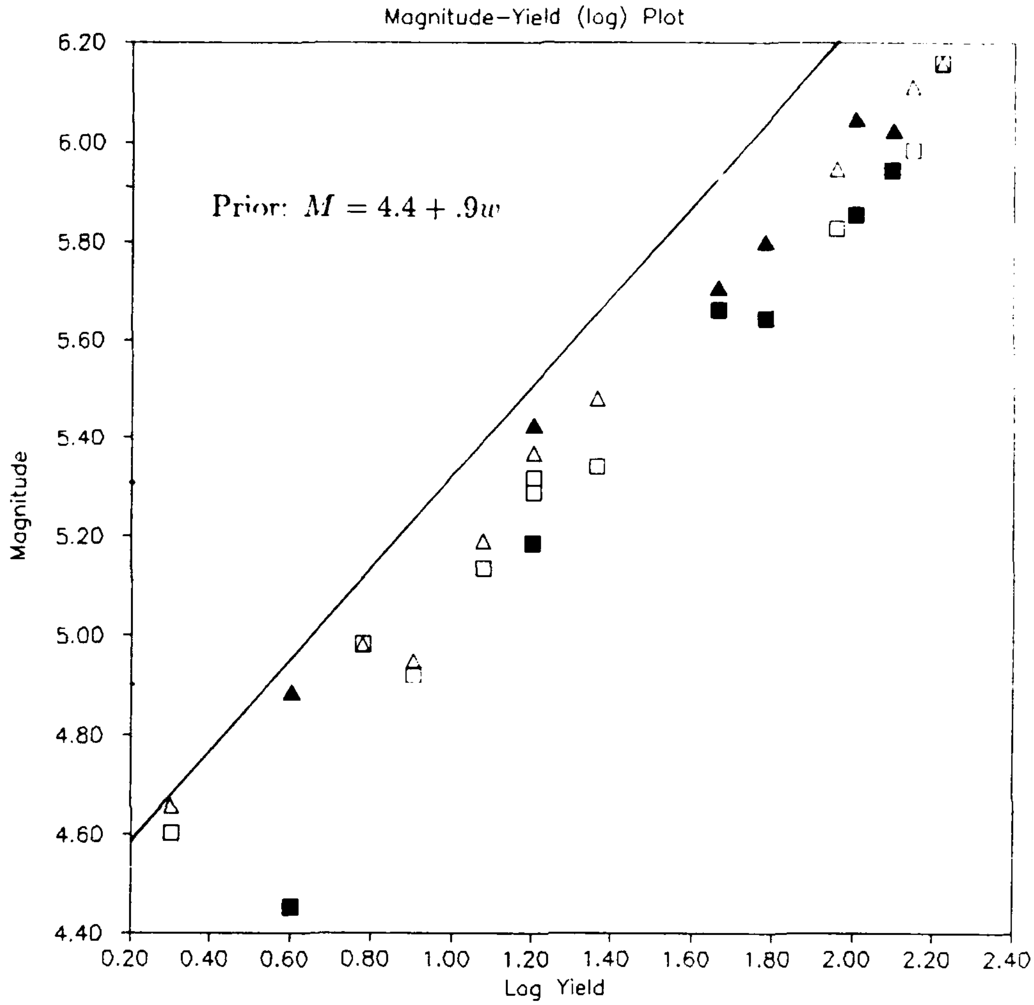

Figure 1: Magnitude-Yield Relations for m_b (squares) and L_g (triangles from 16 Semipalatinsk Explosions. Calibration events are shaded. Prior Regression line $a_0 = 4.4, b_0 = .9$.

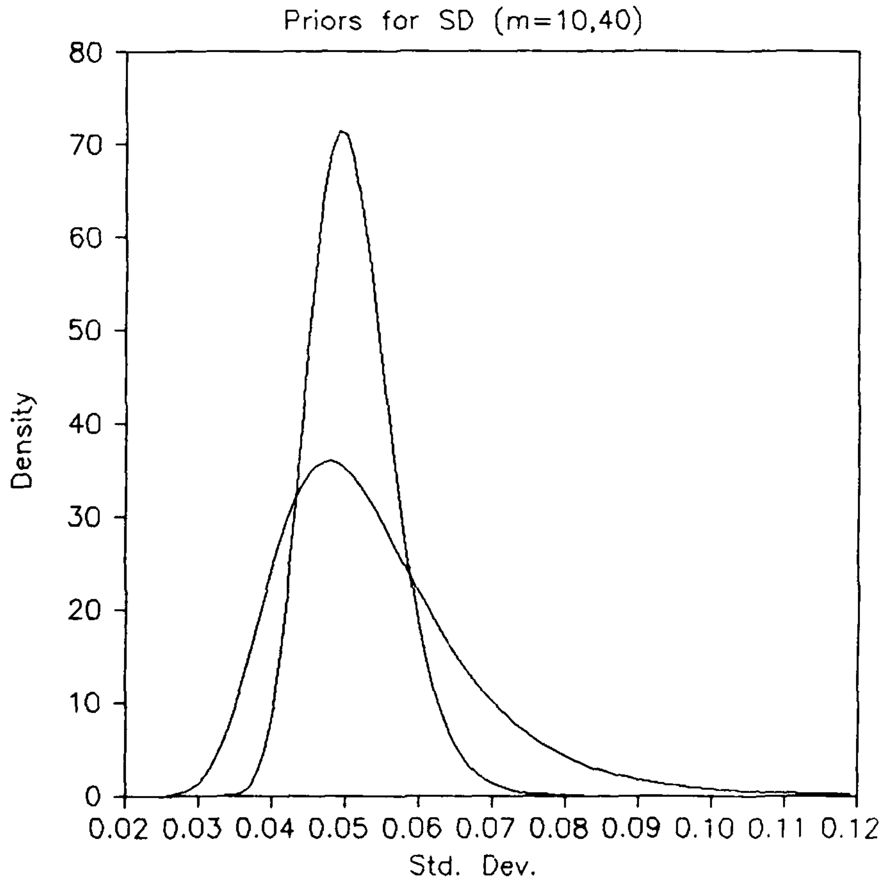

Figure 2: Prior Probability Distributions for Standard Deviation for $\sigma_0 = .05$ (m=10 and 40 degrees of freedom).

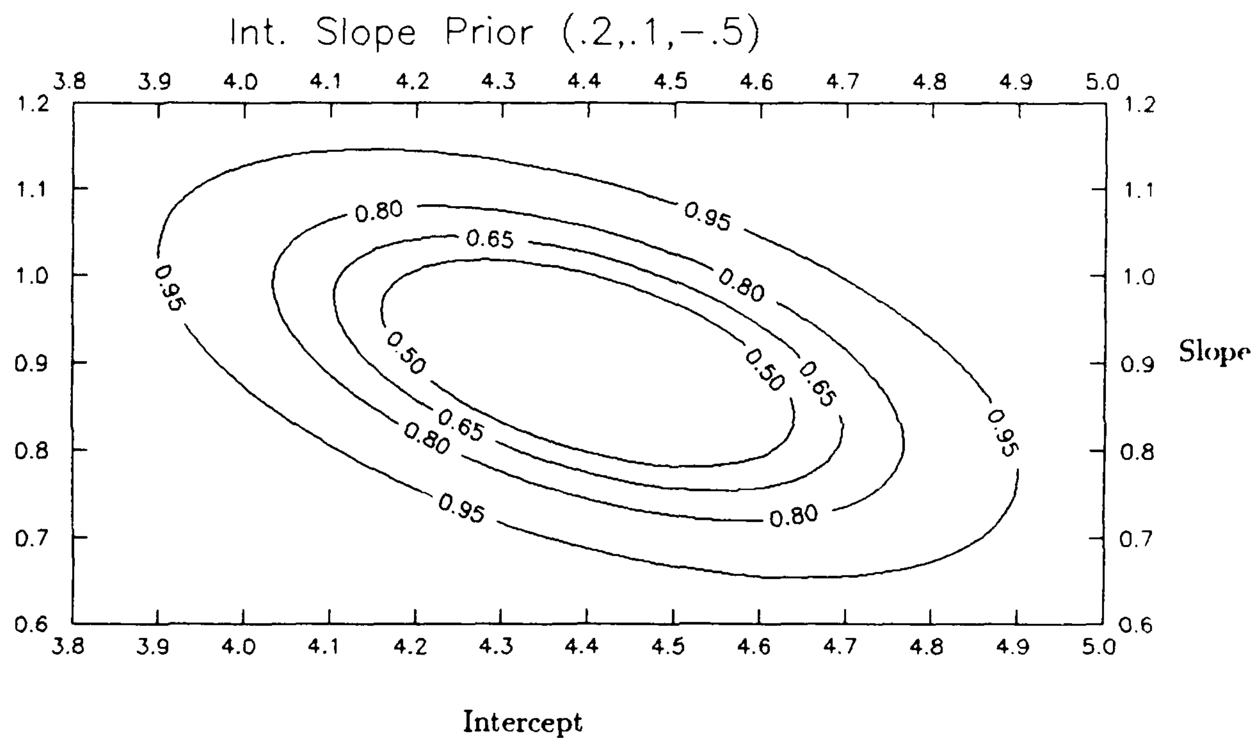

Figure 3: Prior Distribution of Intercept and Slope with $a_0 = 4.4, b_0 = .9, \sigma_a = .2, \sigma_b = .1, \rho_{ab} = -.5$. Contours are cumulative probability that the intercept-slope pair is contained within the region.

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